**Program:** Advanced Scientific Computing Research

**Agency:** Department of Energy

Bureau: Office of Science

Type(s): Research and Development Competitive Grant Capital Assets and Service Acquisitio

 Section Scores
 Overall Rating

 1
 2
 3
 4
 Moderately

 100%
 70%
 67%
 87%
 Effective

Question Weight: 20%

Answer: YES

#### 1.1 Is the program purpose clear?

Explanation: The mission of the Advanced Scientific Computing Research (ASCR) program is to discover, develop, and deploy the computational and networking tools

that enable researchers in the scientific disciplines to analyze, model, simulate, and predict complex phenomena important to the Department of Energy (DOE). To accomplish this mission the program fosters and supports fundamental research in advanced scientific computing applied mathematics,

computer science, and networking and operates supercomputer, networking, and related facilities.

Evidence: FY 2004 Budget Request (www.mbe.doe.gov/budget/04budget/index.htm). Public Law 95-91 that established the Department of Energy (DOE). The

ASCR Mission has been validated by the Advanced Scientific Computing Advisory Committee (ASCAC).

1.2 Does the program address a specific and existing problem, interest or need? Answer: YES Question Weight: 20%

Explanation: The ASCR program addresses the specific need for the Department of Energy's Office of Science (SC) to develop large-scale, complex, high-performance

simulation capabilities to accelerate civilian scientific advancement focused on the mission needs of the DOE, and secondarily on the needs of the

broader scientific community.

Evidence: This program was specifically authorized in the "High Performance Computing Act of 1991" (PL 102-194). The "Scientific Discovery through Advanced

Computing (SciDAC)" plan describes the issues and the program's strategic vision circa 2000 (www.osti.gov/scidac/SciDAC.pdf).

1.3 Is the program designed so that it is not redundant or duplicative of any other Federal, Answer: YES Question Weight: 20%

state, local or private effort?

Explanation: The ASCR program is unique in addressing the specific computational needs and challenges of civilian R&D in the DOE. ASCR is coordinated with

other Federal programs through the Interagency Working Group on IT R&D (IWG/IT R&D) to ensure that efforts are not needlessly redundant. The most recent strategic vision for the program (SciDAC) briefly describes relationships with the computing programs at DOE's National Nuclear Security

Administration and other Federal agencies.

Evidence: IWG/IT R&D (www.itrd.gov/iwg/program.html). SciDAC plan (see above).

1.4 Is the program design free of major flaws that would limit the program's effectiveness or Answer: YES Question Weight: 20%

efficiency?

Explanation: The ASCR program is based on competitive merit-review, independent expert advice, and joint program planning. This proves efficient and effective.

However, a Committee of Visitors (COV) has vet to independently validate ASCR's merit review process.

Evidence: ASCAC reports (www.sc.doe.gov/ascr/adviscommittee.html). Joint planning efforts include SciDAC, Genomes to Life (doegenomestolife.org), and

computational nanoscience (www.sc.doe.gov/production/bes/besac/Theory%20and%20Modeling%20in%20Nanoscience.pdf). Program reviews and files.

Program ID: 10000074

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Program:	Advanced Scientific Computing	Research		Se	ection	Scores		Overall Rating
Agency:	Department of Energy			1	2	3	4	Moderately
Bureau:	Office of Science			100%	70%	67%	87%	Effective
Type(s):	Research and Development	Competitive Grant	Capital Assets and Service	e Acquisitio	)			
1.5	Is the program effectively targe and/or otherwise address the pr	-	each intended beneficiaries	Answer:	YES		Que	stion Weight: 20%
Explanation:	ASCAC ensure that research comm linked to the application programs							
Evidence:	ASCAC reviews and reports. SciDA	C reports (www.osti.gov/scidad	e). Program files.					
2.1	Does the program have a limiter focus on outcomes and meaning			Answer:	YES		Que	stion Weight: 10%
Explanation:	While not comprehensive, the two leads ASCR, and provide a test case for the "minimally effective" performance in update the measures as necessary.	e computation component of th nilestones for each measure, an	ne Genomes to Life SciDAC effort. T and an external panel will assess inte	he program rim prograi	has den n perfe	efined "s ormance	uccessfi on a tri	ıl" and ennial basis, and
Evidence:	SciDAC goals are outlined in progra "successful" and "minimally effectiv (www.sc.doe.gov/measures).							
2.2	Does the program have ambition	us targets and timeframes f	or its long-term measures?	Answer:	YES		Que	stion Weight: 10%
Explanation:	ASCAC has reviewed the new long-computer science, applied mathema		and found them to be ambitious ar	nd meaning	ful ind	icators o	f progre	ess toward
Evidence:	Letter from ASCAC chair regarding	review of long-term measures.						
2.3	Does the program have a limited can demonstrate progress toward			Answer:	YES		Que	stion Weight: 10%
Explanation:	ASCR has developed quantitative at on efficiently providing the computation improved scientific progress.							
Evidence:	FY04 Budget Request. Description of procurement process alluded to in the						n of "be	st value"
2.4	Does the program have baseline	s and ambitious targets for	its annual measures?	Answer:	YES		Que	stion Weight: 10%
Explanation:	All of the annual measures include current rates. Baseline data (FY02 $$							
Evidence:	FY04 Budget Request. Description of (www.nersc.gov/research/annrep02/		o long-term goals (www.sc.doe.gov/n	neasures). I	NERSC	C FY02 A	nnual I	Report

Program:	Advanced Scientific Computing R	Research	5	Se	ection	Scores		Overall Rating
Agency:	Department of Energy			1	2	3	4	Moderately
Bureau:	Office of Science			100%	70%	67%	87%	Effective
Type(s):	Research and Development	Competitive Grant	Capital Assets and Service	Acquisitio	)			
2.5	Do all partners (including grante other government partners) compoals of the program?			Answer:	NO		Que	estion Weight: 10%
Explanation:	ASCR program solicitations for resear grant portfolio that is aimed at the lo "performance expectations generally the labs contain generic "scientific quantum program of the labs contain generic".	ong-term goals of the program. flowed down into the scope of	For contractors, a limited FY03 auwork at the national laboratories."	dit by the l	DOE In	spector	Genera	al (IG) found that
Evidence:	Most recent general renewal solicitate M&O contract performance evaluation BattelleContract.htm; and, Lawrence	on provisions (WWW-accesible	examples include: Oak Ridge Nation	nal Lab, w	ww.orn	l.gov/Co		
2.6	Are independent evaluations of s or as needed to support program to the problem, interest, or need?	improvements and evalua		Answer:	NO		Que	estion Weight: 10%
Explanation:	ASCAC has conducted a fairly light reviews of the research program by a receive the first COV report by April	n independent panel. The pro						
Evidence:	ASCAC facilities review report (www	.krellinst.org/esinfo/ASCAC-fa	acilities-final.mhw.doc).					
2.7	Are Budget requests explicitly tic performance goals, and are the r manner in the program's budget?	esource needs presented in		Answer:	NO		Que	estion Weight: 10%
Explanation:	DOE has not yet provided a budget r	equest that adequately integra	ates performance information.					
Evidence:								
2.8	Has the program taken meaning	ful steps to correct its strat	egic planning deficiencies?	Answer:	YES		Que	estion Weight: 10%
Explanation:	In addition to active participation in workshops, participated in the drafti coordination with OMB. A new COV activity level of ASCAC is below that	ng of a new Office of Science s process is being organized, w	trategic plan, and new performance ith the first program element review	goals and t	targets	have be	en dev	eloped in
Evidence:	Interagency task force (www.itrd.gov applications workshop (www.pnl.gov (www.sc.doe.gov/ascr/ascac_reports.h	/scales). Program files, includ						rkshop). Science

Program:	Advanced Scientific Computin	ng Research		Se	ection S	Scores		Overall Rating
Agency:	Department of Energy			1	2	3	4	Moderately
Bureau:	Office of Science			100%	70%	67%	87%	Effective
Type(s):	Research and Development	Competitive Grant	Capital Assets and Service	Acquisition	)			
2.CA1	Has the agency/program cond that includes trade-offs betwee results to guide the resulting	en cost, schedule, risk, and pe	redible analysis of alternatives or formance goals and used the	Answer:	YES		Que	stion Weight: 10%
Explanation:		ughly equivalent analyses, which	of alternatives analysis as other cap typically compare the attributes of v ision.					
Evidence:	Brief description of "best value" p www.nersc.gov/research/annrep0		ion facility, National Energy Resear	ch Scientii	fic Com	puting (	Center	(NERSC,
2.RD1	If applicable, does the program the program to other efforts t		ential benefits of efforts within	Answer:	NA		Que	stion Weight: 0%
Explanation:	This is a basic R&D program, and	d the question is intended for indu	stry-related R&D programs.					
Evidence:								
2.RD2	Does the program use a priori decisions?	itization process to guide bud	get requests and funding	Answer:	YES		Que	stion Weight: 10%
Explanation:	planwith the input of external co	ommunity workshopsas a part o C programs. However, the progra	practices include a priority ranking f the overall SC planning process. As am has not yet fully engaged ASCAC thin a prioritization framework.	SCR has er	ngaged	the advi	isory pı	ocess for the
Evidence:	ASCAC reports (www.sc.doe.gov/a advisory processes include: Genor (www.sc.doe.gov/production/bes/b	mes to Life (doegenomestolife.org)		b site). Er	ngagem	ent with	other	SC programs
3.1	Does the agency regularly colinformation from key program performance?		rmance information, including ge the program and improve	Answer:	NO		Que	stion Weight: 8%
Explanation:	and national labs, and uses peer in process, such as regular COV eva	review as a type of standardized of luations, that conducts research p for performance reporting, and the	mance information. The program con uality control at the individual gran portfolio quality and process validation are IG periodically conducts limited re a reported by DOE contractors.	t level. Ho ons. While	wever, DOE IO	there is G contra	not ye acts wit	t a systematic h an outside
Evidence:			bout, www.es.net, www.ccs.ornl.gov/ence.doe.gov/production/grants/605-		ml). Pr	ogram f	iles, inc	cluding peer

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Program:	Advanced Scientific Computing	Research		Se	ection S	Scores		<b>Overall Rating</b>	3
Agency:	Department of Energy			1	2	3	4	Moderately	
Bureau:	Office of Science			100%	70%	67%	87%	Effective	
Type(s):	Research and Development	Competitive Grant	Capital Assets and Service	e Acquisitio	)				
3.2	Are Federal managers and prog contractors, cost-sharing partn cost, schedule and performance	ers, and other government		Answer:	YES		Que	stion Weight: 89	%
Explanation:			ce Plans are directly linked to progrance measures linked to program go						
Evidence:	Program and personnel files. For p (www.science.doe.gov/grants/#Gran		nts on M&O contracts, see evidence	for question	n 2.5. G	rant rul	es for r	enewals	
3.3	Are funds (Federal and partner purpose?	es') obligated in a timely man	nner and spent for the intended	Answer:	YES		Que	stion Weight: 89	%
Explanation:			rogress toward obligating funds con l purposes. SC programs consistent						е
Evidence:	Program files. DOE-wide audit rep	orts.							
3.4	Does the program have procedimprovements, appropriate inceffectiveness in program execu	entives) to measure and ach	<u> </u>	Answer:	YES		Que	stion Weight: 89	%
Explanation:			tening organizational structure and e system performance measures used						
Evidence:		rsc/presentations/Sc99/SC99Kr	asures" tab for the programmatic eff amer6/SC99Kramer6.PPT, and hpcf						
3.5	Does the program collaborate a	and coordinate effectively w	ith related programs?	Answer:	YES		Que	stion Weight: 89	%
Explanation:	primarily with national security ag	encies as oppposed to other civ	collaborations with other programs i ilian science agencies. ASCR is a lead ad Technology Council, including co-	ading agenc	y in the	ongoin	g gover	nmental	
Evidence:	Summary of joint activities with ot	her agencies (www.sc.doe.gov/a	scr/hitchcock.ppt). Interagency Wor	king Group	on IT l	R&D (w	ww.itrd	.gov/iwg).	

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Program:	Advanced Scientific Computing	g Research		S	ection	Scores		Overall Rating
Agency:	Department of Energy			1	2	3	4	Moderately
Bureau:	Office of Science			100%	70%	67%	87%	Effective
Type(s):	Research and Development	Competitive Grant	Capital Assets and Ser	vice Acquisit	io			
3.6	Does the program use strong f	inancial management practic	es?	Answer	: YES		Que	stion Weight: 8%
Explanation:	SC staff execute the ASCR progra external groups and modified as re			es and practic	es. Thes	e policie	s have	been reviewed by
Evidence:	Various Departmental manuals.	Program files. Audit reports.						
3.7	Has the program taken meaning	ngful steps to address its man	agement deficiencies?	Answer	: YES		Que	stion Weight: 8%
Explanation:	$\operatorname{SC}$ is currently reengineering to in element review expected back by $A$		iciency. A new COV process is b	eing organize	d by AS	CR, wit	h the fi	rst program
Evidence:	SC reengineering information (www.schedule.	w.screstruct.doe.gov). COV char	rge letter to ASCAC chair, includ	ling scope, co	nflict of	interest	issues,	and future
3.CA1	Is the program managed by macapability/performance characterists			Answer ls?	: YES		Que	stion Weight: 8%
Explanation:	Procurement contracts with complifetime of the contract.	uter vendors tie payments to spe	cific deliverables, including the s	sustained syst	em perf	ormance	e measu	ared over the
Evidence:	Exhibit 300s submitted to OMB.	Program files, including competit	ive performance proposals from	vendors.				
3.CO1	Are grants awarded based on a assessment of merit?	a clear competitive process th	at includes a qualified	Answer	: NO		Que	stion Weight: 8%
Explanation:	First time grant applications are entry Investigator (ECPI) program, and not yet been validated by a COV.							
Evidence:	There were 26 new and 9 renewed programs for SciDAC & Microbial $$				intees ir	FY200	1 (inclu	des new
3.CO2	Does the program have oversigactivities?	ght practices that provide suf	ficient knowledge of grantee	Answer	: YES		Que	stion Weight: 8%
Explanation:	In addition to grantee progress resite visits.	ports, program managers stay in	contact with grantees through e	mail and tele	phone, a	nd cond	uct pro	gram reviews and
Evidence:	Reporting requirements for grants site visits, etc.	(www.science.doe.gov/productio	n/grants/605-19.html). Program	files, includin	g docun	nentatio	n of pro	gram manager

**Program:** Advanced Scientific Computing Research **Section Scores Overall Rating** Agency: 1 2 4 Department of Energy Moderately 67% 87% 100% 70% **Bureau:** Effective Office of Science Type(s): Research and Development Competitive Grant Capital Assets and Service Acquisitio 3.CO3 Answer: NO Question Weight: 8% Does the program collect grantee performance data on an annual basis and make it available to the public in a transparent and meaningful manner? Explanation: In accordance with DOE Order 241.1A, the final and annual technical reports of program grantees are made publicly available on the web through the Office of Scientific and Technical Information's "Information Bridge". However, program-level aggregate data on the impact of the grants program is not adequately communicated in the annual DOE Performance and Accountability report. Evidence: DOE Order 241.1A. Information Bridge (www.osti.gov/bridge/), FY02 Performance and Accountability Report (www.mbe.doe.gov/ stratmgt/doe02rpt.pdf). Answer: NO Question Weight: 8% 3.RD1 For R&D programs other than competitive grants programs, does the program allocate funds and use management processes that maintain program quality? Explanation: ASCAC facility reviews, facility steering committees, and user surveys validate the quality of the scientific user facilities. Unsolicited field work proposals from the Federal Labs are merit reviewed, but not competed. The funds for research programs and scientific user facilities at the Federal Labs are allocated through a limited competition analogous process to the unlimited process outlined in 10 CFR 605. However, the quality of the research funded via this process has not vet been validated by a COV. Evidence: ASCAC facility report (www.krellinst.org/esinfo/ASCAC-facilities-final.mhw.doc). Unsolicited proposals (See 10CFR600.6, professionals.pr.doe.gov/ma5/MA-5Web.nsf/FinancialAssistance/Part+600). Example of lab solicitation, with field work proposal reference (www.science.doe.gov/grants/LAB03 17.html). Merit Review procedures (www.sc.doe.gov/production/grants/merit.html). 10 CFR 605 (www.science.doe.gov/production/grants/605index.html). Facility user surveys and user groups/committees (hpcf.nersc.gov/about, www.es.net, www.ccs.ornl.gov/CHUG.html). Program files, including peer review of the facilities. Answer: LARGE Question Weight: 20% Has the program demonstrated adequate progress in achieving its long-term performance 4.1 **EXTENT** goals? Explanation: ASCAC will evaluate progress toward the new long term performance measures every three years, but no external portfolio-level reviews are available other than the generaly positive facilities report by ASCAC. Early results indicate that the SciDAC effort appears to be successful, which is important for acheiving the future goals of the program. Evidence: ASCAC facilities review report (www.krellinst.org/esinfo/ASCAC-facilities-final.mhw.doc). SciDAC update at latest ASCAC meeting (www.sc.doe.gov/ascr/Laub031403.ppt). Answer: YES Question Weight: 20% 4.2 Does the program (including program partners) achieve its annual performance goals? Explanation: Although the three annual performance goals for FY05 are new, ASCR has met the targets for most of its former annual measures. Evidence: FY02 Performance and Accountability Report (www.mbe.doe.gov/ stratmgt/doe02rpt.pdf). FY04 Annual Performance Plan (www.mbe.doe.gov/budget/04budget/content/perfplan/perfplan.pdf).

**Program:** Advanced Scientific Computing Research **Section Scores Overall Rating** Agency: 1 2 4 Department of Energy Moderately 67% 87% 100% 70% **Bureau:** Effective Office of Science Research and Development Competitive Grant Capital Assets and Service Acquisitio Type(s): 4.3 Answer: YES Question Weight: 20% Does the program demonstrate improved efficiencies or cost effectiveness in achieving program goals each year? Explanation: The sustained system performance metric used by NERSC for procurements has resulted in machines with more compute nodes delivered by the vendor than originally planned, which in turn allows more scientific simulations to be carried out. Evidence: Program files, including procurement contracts. Answer: NA Question Weight: 0% 4.4 Does the performance of this program compare favorably to other programs, including government, private, etc., with similar purpose and goals? Explanation: While user surveys regularly show a fairly high level of satisfaction with ASCR facilities, expert comparitive analyses of the program as a whole have not been done. The program has a unique role to serve the needs of the other five SC research programs, and the DOE mission more broadly, so the value of such analyses is questionable at best given the interconnectedness of the U.S. computing community. Evidence: NERSC Annual User Survey (hpcf.nersc.gov/about/survey/). Answer: LARGE Question Weight: 20% 4.5 Do independent evaluations of sufficient scope and quality indicate that the program is **EXTENT** effective and achieving results? Explanation: The ASCR facilities are effective in achieving desired results, based on assessment by the ASCAC in their facilities report, and based on external peer review of both NERSC and ESnet. However, no independent review process has been carried out to assess the program's research portfolio. ASCAC facilities review report (www.krellinst.org/esinfo/ASCAC-facilities-final.mhw.doc). Program files, including ESnet and NERSC peer review Evidence: results. 4.CA1 Answer: YES Question Weight: 20% Were program goals achieved within budgeted costs and established schedules? Explanation: Performance data for FY02 and FY03 demonstrate that the capital asset procurements, primarily for NERSC acquisitions, were almost exactly on schedule and on budget. This excellent performance can be primarily attributed to the sustained system performance metric used for these procurements, which focuses on the actual performance of the resource available to the end users rather than on the theoretical performance of a proposed system. Evidence: Exhibit 300s submitted to OMB. FY02 Performance and Accountability Report (www.mbe.doe.gov/stratmgt/doe02rpt.pdf). Brief description of "best value" procurement for NERSC (www.nersc.gov/research/annrep01/03systems.html#NERSC4).

#### PART Performance Measurements

**Program:** Advanced Scientific Computing Research

**Agency:** Department of Energy

**Bureau:** Office of Science

Measure:

Progress toward developing the mathematics, algorithms, and software that enable scientifically-critical models of complex systems, including highly nonlinear or uncertain phenomena, or processes that interact on vastly different scales, or contain both discrete and continuous elements. An independent expert panel will conduct a review and rate progress (excellent, adequate, poor) on a triennial basis.

Additional

An external panel will conduct triennial reviews of progress. See www.sc.doe.gov/measures for more information.

**Information:** 

Year	<u>Target</u>	<u>Actual</u>	Measure Term:	Long-term
2006	Excellent			
2009	Excellent			
2012	Excellent			
2015	Excellent			

Measure:

Progress toward developing, through the Genomes to Life partnership with the Biological and Environmental Research program, the computational science capability to model a complete microbe and a simple microbial community. An independent expert panel will conduct a review and rate progress (excellent, adequate, poor) on a triennial basis.

Additional Information:

 $An \ external \ panel \ will \ conduct \ triennial \ reviews \ of \ progress. \ See \ www.sc.doe.gov/measures \ for \ more \ information.$ 

<u>Year</u>	<u>Target</u>	<u>Actual</u>	Measure Term:	Long-term
2006	Excellent			
2009	Excellent			
2012	Excellent			
2015	Met Goal			

Measure:

Focus usage of the primary supercomputer at the National Energy Research Scientific Computing Center on capability computing (percentage of the computing time used that is accounted for by computations that require at least 1/8 of the total resource).

Additional Information:

There were two primary supercomputers, in different lifecycle stages, at the Center in 2002. See www.sc.doe.gov/measures for more information.

<u>Year</u>	<u>Target</u>	<u>Actual</u>	Measure Term: Annual
2002		75%, 22%	

#### **PART Performance Measurements**

**Program:** Advanced Scientific Computing Research

**Agency:** Department of Energy

Bureau: Office of Science

**Measure:** 

Focus usage of the primary supercomputer at the National Energy Research Scientific Computing Center on capability computing (percentage of the computing time used that is accounted for by computations that require at least 1/8 of the total resource).

Additional

There were two primary supercomputers, in different lifecycle stages, at the Center in 2002. See www.sc.doe.gov/measures for more information.

**Information:** 

<u>Year</u>	<u>Target</u>	<u>Actual</u>	<b>Measure Term:</b>
2003		36%	
2004	50%		
2005	50%		

Measure:

Maintain Procurement Cost/Performance Baselines. Percentages within: (1) original baseline cost for completed procurements of major computer systems or network services; and, (2) original performance baseline versus integrated performance over the life of the contract(s).

Additional

See www.sc.doe.gov/measures for more information.

**Information:** 

<u>Year</u>	<u>Target</u>	<u>Actual</u>	<b>Measure Term:</b>	Annual
2002	<10%, <10%	0%, 0%		
2003	<10%, <10%	0%, -1%		
2004	<10%, <10%			
2005	<10%, <10%			

**Measure:** 

Improve Computational Science Capabilities. Average annual percentage increase in the computational effectiveness (either by simulating the same problem in less time or simulating a larger problem in the same time) of a subset of the application codes within the Scientific Discovery through Advanced Computing effort.

Additional Information:

 $Initial\ baseline\ set\ against\ 2002.\ See\ www.sc.doe.gov/measures\ for\ more\ information, including\ the\ declaration\ of\ the\ subset\ of\ application\ codes.$ 

<u>Year</u>	<u>Target</u>	<u>Actual</u>	Measure Term: Annual	(Efficiency Measure)
2003	10%	3181%		
2004	50%			
2005	50%			

Program ID: 10000074

Annual